

Se-(8-Azidoadenosyl)selenomethionine

135608-83-2 | DTXSID70159478

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: -10.2 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 7.33e-02

Confidence level: 8.74e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Isoproturon

Measured: -10.9

Predicted: -10.5

[Image not found](#)

alpha-Humulene

Measured: -9.54

Predicted: N/A

[Image not found](#)

Cyclopropaneacetaldehyde,
2,2-dimethyl-3-(2-oxopropyl)-

Measured: -10.3

Predicted: -10.3